

Nonequilibrium quantum decay and decoherence in quantum impurity problems

Holger Baur¹, Andrea Fubini², and Ulrich Weiss¹

¹*Institut für Theoretische Physik, Universität Stuttgart, D-70550 Stuttgart, Germany and*

²*Dipartimento di Fisica, Università di Firenze, and INFN,*

UdR Firenze, Via G.Sansone 1, I-50019 Firenze, Italy

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Abstract

Using detailed balance and scaling properties of integrals that appear in the Coulomb gas reformulation of quantum impurity problems, we establish exact relations between the nonequilibrium quantum decay rates of the boundary sine-Gordon and the anisotropic Kondo model at zero temperature. Combining these results with findings from the thermodynamic Bethe ansatz, we derive exact closed form expressions for the quantum decay rate of the dissipative two-state system in the scaling limit. These expressions illustrate how the crossover from weak to strong tunneling takes place. We trace out the regimes in which the usually applied Golden Rule (nonadiabatic) rate expression fails. Using a conjectured correspondence between the relaxation and dephasing rate, we obtain the exact lower bound of the dephasing rate as a function of bias and dissipation strength.

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Quantum impurity problems (QIPs) have attracted a great deal of interest recently. This is because the underlying physics is non-trivial and the models are manageable technically despite their essentially nonperturbative nature. In addition, they have a multitude of experimental applications, including the Kondo effect, quantum dots, dissipative quantum mechanics, tunneling in quantum wires and fractional quantum Hall devices [1].

There have been discovered various relations between thermodynamic quantities of the anisotropic Kondo model (AKM) and the boundary sine-Gordon (BSG) field theory model [2]. Each of these integrable models is of considerable interest and it is remarkable that they are closely related. The AKM corresponds to the dissipative two-state system (TSS) in the Ohmic scaling limit [3] and the BSG model corresponds to the Schmid model [4]. The latter describes a quantum Brownian particle coupled to an Ohmic heat bath and moving in a tilted cosine potential. The tight-binding (TB) limit of the Schmid model is equivalent to the strong-backscattering limit of the BSG model, while the weak-binding (WB) limit of the Schmid model represents the weak-backscattering limit of the BSG model. In the sequel, we use the language of dissipative quantum mechanics.

The equivalence or difference of these models can most easily be seen in the Anderson-Yuval Coulomb gas representation for the partition function. The partition function of all these models can be expressed as the partition function of a one-dimensional classical gas of positive and negative unit charges with "log-sine" interactions. The AKM (or TSS) problem differs from the BSG (or Schmid) model by a different ordering prescription.

In this Letter, we calculate the full nonequilibrium quantum decay rate of the TSS at zero temperature in closed analytic form. Upon using a conjectured correspondence between relaxation and decoherence in the TSS, we also determine the lower bound for decoherence in this system. These outstanding problems are solved by establishing exact functional relations between nonequilibrium quantum rates of the TSS and the Schmid model.

The TSS Hamiltonian in pseudospin form reads

$$H_{\text{TSS}} = -\frac{1}{2}\Delta_{\text{T}}\sigma_x - \frac{1}{2}[\epsilon + f(t)]\sigma_z,$$

where $\hbar = k_{\text{B}} = 1$. Here Δ_{T} is the tunneling coupling, ϵ is the bias energy, and $f(t)$ is a random force with Gaussian statistics. All effects of $f(t)$ are captured by the second integral of the force autocorrelation function, denoted by $Q(t)$. In the scaling (or field theory) limit, we have $Q(t) = 2K \ln[(\omega_c/\pi T) \sinh(\pi T|t|)] + i\pi K \text{sgn}(t)$, where T is temperature and ω_c is

a cut-off frequency. The Kondo parameter K is a dimensionless Ohmic damping strength, which is the inverse of the Luttinger parameter g or the filling fraction ν in quantum impurity problems.

The TB Schmid model in second quantized form with coupling energy Δ_S and bias energy ϵ is given by

$$H_S = -\frac{1}{2}\Delta_S \sum_n (a_n^\dagger a_{n+1} + \text{h.c.}) - [\epsilon + f(t)] \sum_n n a_n^\dagger a_n .$$

The nonequilibrium dynamics of both models may be computed using the Keldysh or Feynman-Vernon formalism for the reduced density matrix (RDM). Consider a particular path on the (q, q') -plane of the RDM parametrized by charges $\{u_j = \pm 1\}$ and $\{v_i = \pm 1\}$ chronologically arranged on the q and q' path, respectively. The influence functional due to the stochastic force $f(t)$ for k charges on the q -path and ℓ charges on the q' -path, divided up into the self-interactions of the paths and the interaction between the paths, reads

$$\begin{aligned} \mathcal{F} = \exp & \left\{ \sum_{j>i=1}^k u_j u_i Q(t_j - t_i) \right. \\ & \left. + \sum_{j>i=1}^\ell v_j v_i Q^*(t'_j - t'_i) - \sum_{j=1}^\ell \sum_{i=1}^k v_j u_i Q(t'_j - t_i) \right\} . \end{aligned}$$

For the TSS the charges u_j, v_i alternate in sign, while for the Schmid model they may be ordered arbitrarily. At long times, the Schmid model is a Poissonian transport model: the population dynamics results from uncorrelated direct forward and backward transitions by n wells, $n = 1, 2, \dots$. Since they are not classical, the respective weights per unit time (“rates”) γ_n^\pm are not necessarily positive because of quantum interference [5]. In the TB representation, the Fourier transform of the population distribution $\hat{P}(k, t) = \sum_n e^{ikn} P_n(t)$ takes the form $\hat{P}(k, t) = \prod_{n=1}^\infty \exp [t (e^{ikn} - 1) \gamma_n^+ + t (e^{-ikn} - 1) \gamma_n^-]$, where the rates γ_n^\pm describe uncorrelated direct forward/backward transitions by n TB states.

The Poissonian dynamics is found upon carrying out a cluster decomposition of the individual path contributions to the Laplace transform $\hat{P}(k, \lambda)$ in the limit $\lambda \rightarrow 0$. A cluster is a λ -independent (irreducible) path section which starts and ends in a diagonal state of the RDM, $\sum_i u_i = \sum_j v_j$ and cannot be factorized into clusters of lower order. By definition, the clusters are noninteracting. Therefore a succession of clusters factorizes and the integral over a (time) interval separating any two clusters produces a factor $1/\lambda$. Path segments which start and end in a diagonal state and again have interim visits of diagonal states

are reducible, i.e. they factorize into clusters of lower order and factors of $1/\lambda$. However, after subtraction of all the reducible components, an irreducible part is left. The irreducible contributions of all charge arrangements with excess charge $\sum_j u_j = \pm n$, $\sum_i v_i = \pm n$ define the transition rates γ_n^\pm .

The irreducible parts of arrangements with $2(n + \ell + k)$ charges contribute to the order $\Delta^{2(n+\ell+k)}$ of γ_n^+ . They can be divided into a multitude of different subsets. Each subset α is a particular arrangement of $n + 2\ell$ time-ordered u -charges and $n + 2k$ time-ordered v -charges. The number of subsets with different order of the u - and v -charges is $N = N_u N_v = \frac{(n+2\ell)!}{\ell!(n+\ell)!} \frac{(n+2k)!}{k!(n+k)!}$. In each individual subset α , all possible orders of the u -charges relative to the v -charges are taken into account, which amounts to $N_{u,v} = \frac{(2n+2\ell+2k)!}{(n+2\ell)!(n+2k)!}$ different arrangements. Each subset α defines a partial forward rate $\gamma_n^{\alpha,+}$. The corresponding partial backward rate $\gamma_n^{\alpha,-}$ is represented by the arrangement with reverse order and reverse sign of the charges. The individual partial rates are directly related by detailed balance, $\gamma_n^{\alpha,-} = e^{-n\epsilon/T} \gamma_n^{\alpha,+}$. Detailed balance is satisfied for every partial rate because the interaction $Q(z)$ between the u - and v -charges is analytic for complex time z in the strip $0 \geq \text{Im } z > -1/T$ and has the property $Q(t - i/T) = Q^*(t)$.

In the remainder, we restrict the attention to zero temperature. At $T = 0$, all frequencies of the Schmid and TSS model can be absorbed into a single dimensionless parameter, $x_S = (\epsilon/\omega_c)^K \Delta_S/\epsilon$ and $x_T = (\epsilon/\omega_c)^K \Delta_T/\epsilon$. For later convenience we also introduce the frequency scale ϵ_0 (analogous to the Kondo scale in the Kondo model and the scale T'_B in QIPs [6]) and the dimensionless bias $v = \epsilon/\epsilon_0$. The scale ϵ_0 is related to the bare parameters of the Schmid and TSS model as [1]

$$\epsilon_0^{2-2K} = \frac{2^{2-2K} \pi^2}{\Gamma^2(K)} \frac{\Delta_S^2}{\omega_c^{2K}}, \quad \epsilon_0^{2-2K} = \frac{\Gamma^2(1-K)}{2^{2K}} \frac{\Delta_T^2}{\omega_c^{2K}}.$$

In the scale ϵ_0 , the selfduality of the BSG model becomes evident. In the second form, we have anticipated from below, that at fixed ϵ_0 the TSS bare coupling Δ_T is related to the BSG bare coupling Δ_S via $\Delta_T = 2 \sin(\pi K) \Delta_S$ [2].

The rates of the Schmid model can be written as [5]

$$\gamma_n^\pm = \epsilon \sum_{\ell=n}^{\infty} x_S^{2\ell} U_{n,\ell}^\pm. \quad (1)$$

To proceed, we map the u - and v -charges onto a single time axis. To this end, we introduce charges $\eta_j = \pm 1$ describing forward/backward moves along the quasiclassical path $q + q'$

and charges $\xi_j = \pm 1$ representing moves along the quantum fluctuation path $q - q'$. The cumulative charge $p_\ell = \sum_{k=1}^\ell \xi_k$ measures how far the system is off-diagonal after ℓ moves. Then we have

$$U_{n,\ell}^\pm = \frac{1}{2^{2\ell}} \sum_{\{\xi_j\}'} \sum_{\{\eta_i\}'} [\cos \phi_\ell I_\ell^+ \pm \sin \phi_\ell I_\ell^-] . \quad (2)$$

Here $\{\dots\}'$ denotes the constraints $\sum_j \xi_j = 0$ for the 2ℓ ξ -charges and $\sum_i \eta_i = 2n$ for the 2ℓ η -charges. The number of different charge sequences contributing to $U_{n,\ell}^\pm$ is $N_{\xi,\eta} = \frac{(2\ell)!}{\ell! \ell!} \frac{(2\ell)!}{(\ell+n)!(\ell-n)!}$. The imaginary parts of the bath correlations in the influence functional \mathcal{F} add up to the influence phase $\phi_\ell(\vec{\xi}, \vec{\eta}) = \pi K \sum_{j=1}^{2\ell-1} p_j \eta_j$.

All the quantum fluctuations are in the $2\ell-1$ -fold integrals I_ℓ^\pm , which are independent of $\vec{\eta}$. With the notation $\int_0^\infty \mathcal{D}_{2\ell-1}(\vec{\tau}) \dots \equiv \int_0^\infty d\tau_{2\ell-1} \dots d\tau_1 \dots$, where the τ_j are the dimensionless charge intervals (scaled with ϵ), we get

$$I_\ell^+(\vec{\xi}) \pm i I_\ell^-(\vec{\xi}) \equiv \int_0^\infty \mathcal{D}_{2\ell-1}(\vec{\tau}) G_\ell^{(c)}(\vec{\tau}, \vec{\xi}) e^{\pm i \varphi_\ell(\vec{\tau}, \vec{\xi})} .$$

The bias phases are combined in the phase $\varphi_\ell(\vec{\tau}, \vec{\xi}) = \sum_{j=1}^{2\ell-1} p_j \tau_j$. The interactions of the ξ -charges are encapsulated in the factor (we put $\tau_{ji} = t_j - t_i = \sum_{k=i}^{j-1} \tau_k$)

$$G_\ell^{(c)}(\vec{\tau}, \vec{\xi}) = \exp \left(2K \sum_{j>i=1}^{2\ell} \xi_j \xi_i \ln \tau_{ji} \right) - G_\ell^{(\text{subtr})}(\vec{\tau}, \vec{\xi}) .$$

The subtractions are to ensure that the I_ℓ^\pm represent irreducible clusters. Subtractions are needed whenever one or several of the cumulative p -charges are zero. For instance, putting $\ell = 2$ and $\xi_2 = -\xi_1$, $\xi_4 = -\xi_3$ we then have $G_2^{(\text{subtr})} = (\tau_1 \tau_3)^{-2K}$.

The expression for $U_{n,\ell}^\pm$ can be simplified considerably upon utilizing the following observations:

(i) At $T = 0$, backward moves to higher wells are absent, i.e. the aforescribed partial backward rates $\gamma_n^{\alpha,-}$ are all zero. Hence for any subset α , the respective linear combination of the I_ℓ^+ -integrals cancels that of the I_ℓ^- -integrals, while they add up in $\gamma_n^{\alpha,+}$.

(ii) For every individual $\vec{\xi}$ -configuration, in which all cumulative charges p_j have the same sign (some of them may be zero), the integrals I_ℓ^\pm are simply related by $I_\ell^+(\vec{\xi}) = \tan(2\pi K \ell) I_\ell^-(\vec{\xi})$.

Property (i) is of general nature since it is due to detailed balance. Property (ii) is based on the scale invariant logarithmic charge interaction in $G_\ell^{(c)}$ and is responsible for

integrability. It does not hold when scale invariance is broken by finite cutoff or finite temperature.

Upon exploitation of properties (i) and (ii) a multitude of linear functional relations between the various integrals $I_\ell^\pm(\vec{\xi})$ with different $\vec{\xi}$ but same ℓ can be derived. The analysis yields that all integrals $I_\ell^\pm(\vec{\xi})$ with one or several p_j equal to zero can be expressed in terms of those which have all p_j nonzero. Making use of these relations we find that there are formidable cancellations among the various contributions to $U_{n,\ell}^+$. In particular, the contributions from arrangements with any fixed nonzero number of negative η -charges cancel each other exactly. Thus we have $U_{n,\ell}^+ = 0$ for $\ell > n$. Hence the contributions of all paths which undertake backward moves between virtual intermediate states add up to zero and only the paths with the minimal number of flips $2n$ contribute to the forward rate γ_n^+ . We finally get

$$U_{n,n}^+ = \frac{(-1)^{n-1}}{n} \sum_{\{\xi_j\}'} I_n^-(\vec{\xi}) \prod_{k=1}^{2n-1} \sin(\pi K p_k) . \quad (3)$$

We now turn to the study of the incoherent dynamics in the TSS. The subset of charge sequences in the Schmid model in which both the u - and v -charges alternate in sign defines a partial rate of γ_1^\pm . This partial rate, denoted by $\tilde{\gamma}^\pm$, is the full rate describing incoherent relaxation in the biased TSS. At $T = 0$, the expansion in the number of transitions (fugacity expansion) gives

$$\tilde{\gamma}^\pm = \sum_{\ell=1}^{\infty} \tilde{\gamma}_\ell^\pm ; \quad \tilde{\gamma}_\ell^\pm = \epsilon x_T^{2\ell} W_\ell^\pm , \quad (4)$$

where $W_\ell^\pm = U_{1,\ell}^\pm$, and where the double sum in (2) is subject to the TSS constraints. The η -sum is easily performed, yielding

$$W_\ell^\pm = \left(\frac{-1}{2}\right)^{\ell-1} \cos^\ell(\pi K) \sum_{\{\xi_j\}''} [I_\ell^+ \pm \xi_1 \tan(\pi K) I_\ell^-] .$$

Here $\{\cdot\}''$ denotes the TSS constraint $\xi_{2k} = -\xi_{2k-1}$.

Making again extensive use of properties (i) and (ii), we find that all the partial backward rates $\tilde{\gamma}_n^-$ vanish and that W_n^+ can be expressed in terms of the $I_n^-(\vec{\xi})$ integrals, in which all p_j are nonzero. In the end we find using (3)

$$W_n^+ = (-1)^{n-1} \frac{4 \sin^2(n\pi K)}{[2 \sin(\pi K)]^{2n}} U_{n,n}^+ . \quad (5)$$

Employing relation (5), we can express the partial rate $\tilde{\gamma}_n^+$ of the TSS in terms of the rate γ_n^+ of the Schmid model. At fixed renormalized coupling ϵ_0 we have

$$\tilde{\gamma}_n^+ = (-1)^{n-1} 4 \sin^2(n\pi K) \gamma_n^+ . \quad (6)$$

Upon combining the thermodynamic Bethe ansatz with the Keldysh approach, the rate γ_n^+ has been found as [5]

$$\gamma_n^+ = \frac{(-1)^{n-1}}{n!} \frac{\Gamma(\frac{3}{2})\Gamma(Kn)}{\Gamma[\frac{3}{2} + (K-1)n]} \frac{\epsilon}{2\pi} v^{(2K-2)n} . \quad (7)$$

Use of the relation (6) and the expression (7) gives the partial rate $\tilde{\gamma}_n^+$ in explicit closed form. The perturbative expansion of the full rate $\tilde{\gamma}^+$ of the TSS is found to read

$$\begin{aligned} \tilde{\gamma}^+ &= \frac{\epsilon}{2\sqrt{\pi}} \sum_{m=1}^{\infty} a_m(K) v^{(2K-2)m} , \\ a_m(K) &= \frac{1}{m!} \frac{\Gamma(Km) [1 - \cos(2\pi Km)]}{\Gamma[\frac{3}{2} + (K-1)m]} . \end{aligned} \quad (8)$$

Expression (8) is the weak-tunneling expansion of the TSS. For rational values of K , the series (8) is a linear combination of hypergeometric functions.

In the regime $K < 1$, the perturbative series is absolutely converging for large enough v , i.e. large enough bias. For $K > 1$, (8) is absolutely converging for small enough v , i.e. small enough bias. The leading term is the Golden Rule rate $\tilde{\gamma}_{\text{GR}}^+ = [\pi/2\Gamma(2K)]\epsilon x_{\text{T}}^2$ [1, 3].

An integral representation for $\tilde{\gamma}^+$ is found by writing $\Gamma(Km)/\Gamma[\frac{3}{2} + (K-1)m]$ as a contour integral. Within the radius of convergence of series (8) we can interchange the order of summation and integration, yielding

$$\tilde{\gamma}^+ = \text{Re} \frac{\epsilon}{2\pi i} \int_{\mathcal{C}} \frac{dz}{z} [(z-1-z^K u_2)^{\frac{1}{2}} - (z-1-z^K u_1)^{\frac{1}{2}}] ,$$

where $u_1 = v^{2K-2}$ and $u_2 = e^{i2\pi K} u_1$. The contour \mathcal{C} starts at the origin, circles anti-clockwise around the square-root branch point which is near $1 + u_{1/2}$ for small v^{2K-2} , and returns to the origin. The integral converges for all K and v , not just in the regime where the series (8) does. Therefore it must also yield the asymptotic expansions for small (large) enough v when $K < 1$ ($K > 1$).

The asymptotic expansion for $K < 1$ can be found by changing variable to $y = (u_{1/2}z)^{1/(1-K)}$ and expanding the integrand for small v . The strong-tunneling series is

$$\tilde{\gamma}^+ = \frac{\epsilon}{2\sqrt{\pi}} \sum_{n=0}^{\infty} b_n(K) v^{2n-1} . \quad (9)$$

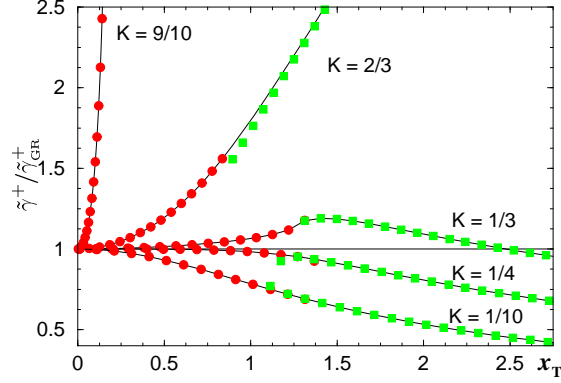


FIG. 1: The scaled rate $\tilde{\gamma}^+/\tilde{\gamma}_{GR}^+$ is plotted versus x_T for various $K < 1$. The circles represent the weak-tunneling series and the squares the strong-tunneling expansion. The full curve is the hypergeometric function expression

For $\frac{1}{3} < K < 1$, the branch cut of the u_2 -term is not encircled by the contour. In this regime we obtain

$$b_n(K) = d_n(K) \equiv \frac{1}{n!} \frac{\Gamma[(\frac{1}{2} - n)\frac{K}{1-K}]}{(\frac{1}{2} - n)\Gamma[(\frac{1}{2} - n)\frac{1}{1-K}]} . \quad (10)$$

For $K \leq \frac{1}{3}$, both the u_1 - and u_2 -term contribute, giving

$$b_n(K) = 2 \sin^2[\frac{\pi K}{1-K}(\frac{1}{2} - n)] d_n(K) . \quad (11)$$

In the limit $K \ll 1$, the perturbative series (8) as well as the asymptotic series (9) can be summed to the known result $\tilde{\gamma}^+ = \pi K \Delta_T^2 / \sqrt{\Delta_T^2 + \epsilon^2}$ [1].

The asymptotic series (9) is an expansion in powers of ϵ^2/ϵ_0^2 . The leading term is independent of ϵ and represents the forward rate for the symmetric TSS,

$$\tilde{\gamma}_0^+ = (2\sqrt{\pi})^{-1} b_0(K) \epsilon_0 , \quad (12)$$

where $b_0(K)$ is given in (10) and (11), respectively.

In Fig. 1, the scaled rate $k^+ \equiv \tilde{\gamma}^+/\tilde{\gamma}_{GR}^+$ is plotted for different $K < 1$. The horizontal line is the $K = \frac{1}{2}$ result. For $K < \frac{1}{4}$, the various tunneling contributions interfere always destructively, which leads to a reduction of the rate. For $\frac{1}{2} < K < 1$, the tunneling contributions interfere constructively for all x_T . In the range $\frac{1}{4} < K < \frac{1}{2}$, the rate goes through a maximum. This reflects constructive interference at small and intermediate x_T , and destructive interference at large x_T .

The nonperturbative result (12) for the relaxation rate may be compared with the decoherence rate γ_{dec} describing damping of the coherent oscillations in the TSS [1]. This rate

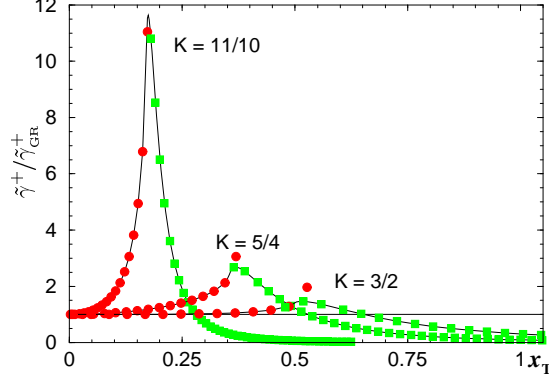


FIG. 2: The same scaled rate, but now for various $K > 1$.

has been calculated for the symmetric TSS in Ref. [7] within the framework of integrable QFT. In our notation, the result is $\gamma_{\text{dec}} = \tilde{\gamma}_0^+ / 2$ for $K \leq \frac{1}{3}$ and $\gamma_{\text{dec}} = \sin^2[\frac{\pi K}{2(1-K)}] \tilde{\gamma}_0^+$ for $\frac{1}{3} < K < \frac{1}{2}$. It is known that the same relations hold for a biased TSS in the regimes $K \ll 1$ and K close to $\frac{1}{2}$ [1]. Upon combining these relations with Eqs. (9) - (11) it is natural to conjecture that the decoherence rate of a biased TSS is

$$\gamma_{\text{dec}} = \frac{\epsilon}{2\sqrt{\pi}} \sum_{n=0}^{\infty} \sin^2[\frac{\pi K}{1-K}(\frac{1}{2} - n)] d_n(K) v^{2n-1}, \quad (13)$$

in agreement with all the known results in special cases. This expression gives the lower ($T = 0$) bound for quantum decoherence in the entire regime $0 < K \leq \frac{1}{2}$.

Finally consider the damping regime $K > 1$ for large v (large bias). By defining the variable $t = e^{-i\pi} u_{1/2} z^K$, we may expand the resulting integrand in powers of $u_{1/2}^{-1/K}$. Introducing the sections $K = p + \kappa$ with $p = 1, 2, \dots$ and $0 \leq \kappa < 1$, we obtain the asymptotic series as

$$\tilde{\gamma}^+ = \frac{\epsilon}{2\sqrt{\pi}} \sum_{m=1}^{\infty} c_m(K) v^{(2/K-2)m}, \quad (14)$$

$$c_m(K) = \frac{(-1)^m}{m!} \frac{2 \Gamma(\frac{m}{K}) \sin[\frac{1+p}{K} m\pi] \sin(\frac{p}{K} m\pi)}{K \Gamma[\frac{3}{2} + (\frac{1}{K} - 1)m]}.$$

This asymptotic series (14) bears a strong resemblance with that of the self-dual Schmid model [6, 8, 9]. The powers follow from those of the perturbative expansion (8) by the substitution $K \rightarrow 1/K$, as also do major parts of the coefficient $c_m(K)$. However, it differs from self-duality by the alternating sign and by the sine-factors.

Fig. 2 gives plots of the scaled rate k^+ for $K > 1$. The rate goes through a maximum which is shifted to higher x_T with increasing K . At large enough x_T , the strong-tunneling contributions interfere always destructively.

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